

Ethanone, 1-(3-hydroxyphenyl)-
121-71-1 | DTXSID5059533

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 108 °C

Global applicability domain: Inside

Local applicability domain index: 8.78e-01

Confidence level: 7.48e-01

Nearest Neighbors from the Training Set

Image not found

Ethanone, 1-(3-hydroxyphenyl)-

Measured: 96.0

Predicted: 108

Image not found

4-Hydroxyacetophenone

Measured: 110

Predicted: 109

Image not found

4-Hydroxy-3-methylbenzaldehyde

Measured: 119

Predicted: 114

Image not found

4-Hydroxy-2-methylacetophenone

Measured: 128

Predicted: 110

Image not found

Benzaldehyde, 3-hydroxy-

Measured: 108

Predicted: 107